

First Steps with UNIX in Life Sciences

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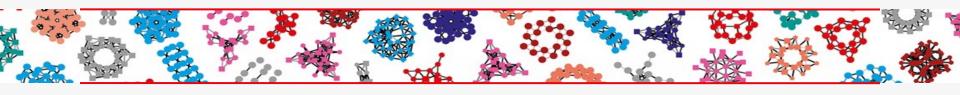




Learning outcomes

- To get familiar with the UNIX environment
- To use the most common UNIX commands
- To acquire skills necessary for further courses requiring UNIX, like HPC and NGS analysis courses.

Outline



- 1. What is UNIX and why should biologists use it?
- 2. UNIX filesystem: navigation and usage
- 3. Environment, processes & Jobs
- 4. Working with directories and files
- 5. Working with file content

Exercises are integrated in chapters

An optional exam will be put online at the end of the course

What is UNIX and why should biologists use it?







Command Line Interface (CLI)

In the 70's, all systems used a command line interface

```
Starting MS-DOS...
C:\>_
```



```
APPLE II

DOS VERSION 3.3 SYSTEM MASTER

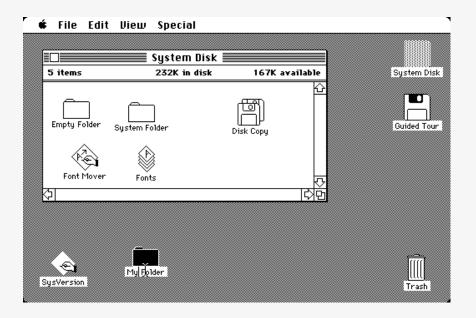
JANUARY 1, 1983

COPYRIGHT APPLE COMPUTER, INC. :980,1982

BESURE WARS COOK STOOMS
```

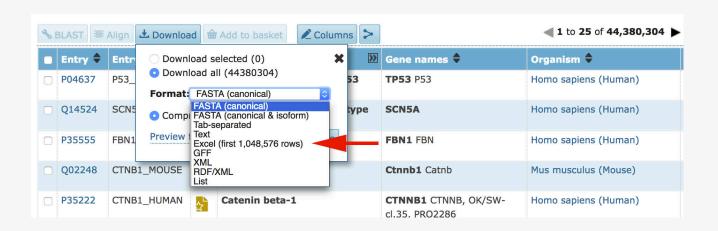
Graphical User Interface (GUI)

- Development since the 60's
- First popular product was the Macintosh in 1984
- **Different way of thinking** / acting: windows, menus, icons, mouse and clicks (now touchscreens)

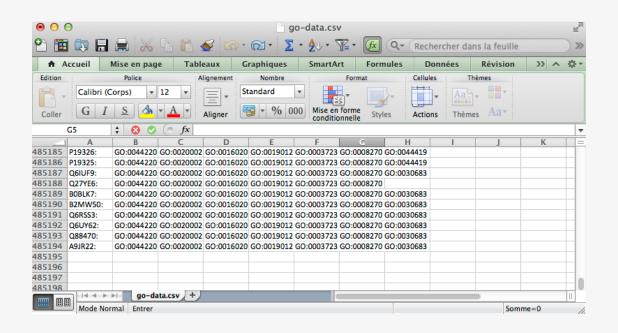


CLI vs GUI – size issues

Dealing with more than 1 million lines



CLI vs GUI - complex queries



- How many Swiss-Prot Identifiers are in the file ?
- How many different GO annotations are there?
- What are the 4 most common GO annotations?

CLI vs GUI - complex queries

How many Swiss-Prot identifiers?

```
userA$ wc -1 go-data.csv
485194
```

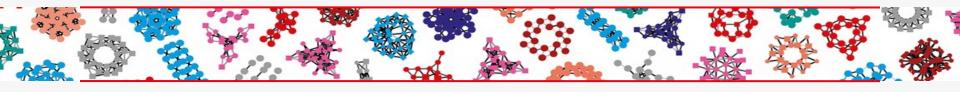
How many different GO annotations?

```
userA$ tr " " "\n" < go-data.csv | grep ^GO: | sort | uniq | wc -1 15696
```

What are the 4 most common GO annotations?

```
userA$ tr " " "\n" < go-data.csv | grep ^GO: | sort | uniq -c |
sort -nr | head -4
127303 GO:0005737
82740 GO:0005524
66591 GO:0016021
52952 GO:0046872</pre>
```

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UNIX filesystem: navigation and usage



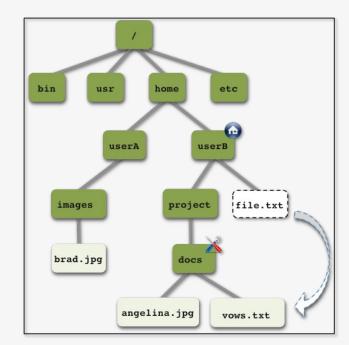


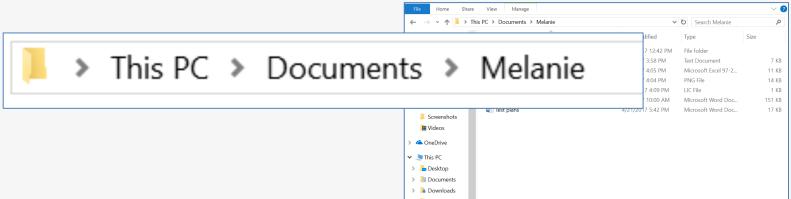


Files & directories

- Organised as an inverted tree
- Single root '/' at the top.
- Directory: is a file containing file & directory names
- Home directory: is the 'private' directory of a user
- Working directory: is the current directory.

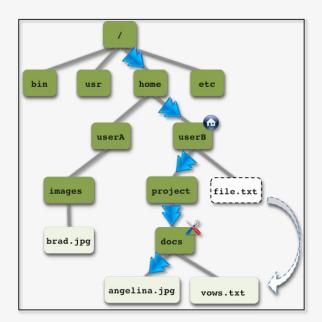
 The one you are in when executing a command.
- File: is a file





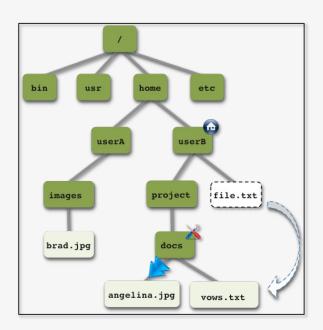
Paths

absolute path...



from the root

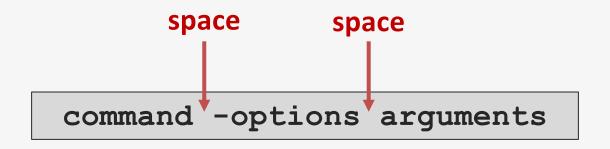
relative path...



from the working directory

angelina.jpg

General command syntax



By default, commands are executed in the working directory

Help about commands & options

man

```
PWD(1)
                          BSD General Commands Manual
                                                                        PWD(1)
NAME
    pwd -- return working directory name
SYNOPSIS
     pwd [-L | -P]
DESCRIPTION
    The pwd utility writes the absolute pathname of the current working directory to the stan-
    dard output.
    Some shells may provide a builtin pwd command which is similar or identical to this util-
     ity. Consult the builtin(1) manual page.
    The options are as follows:
     -L
             Display the logical current working directory.
             Display the physical current working directory (all symbolic links resolved).
    If no options are specified, the -L option is assumed.
ENVIRONMENT
     Environment variables used by pwd:
     PWD Logical current working directory.
EXIT STATUS
    The pwd utility exits 0 on success, and >0 if an error occurs.
SEE ALSO
     builtin(1), cd(1), csh(1), sh(1), getcwd(3)
```

Navigation - Locate

pwd

- for 'print working directory'
- indicates the absolute path of the current directory

```
bin
          usr
                    home
                                etc
                            userB
            userA
                       project
                                  file.txt
   images
  brad.jpg
                        docs
              angelina.jpg
                                vows.txt
```

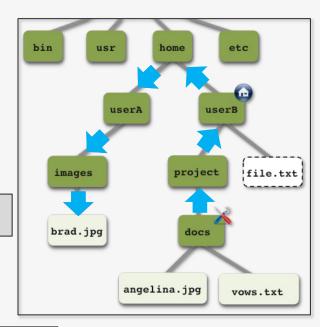
```
userB$ pwd
/home/userB/project/docs
```

Current & parent directories

Example: the current directory is 'docs'

Absolute path to brad.jpg

/home/userA/images/brad.jpg



Relative path to brad.jpg

Parent directory

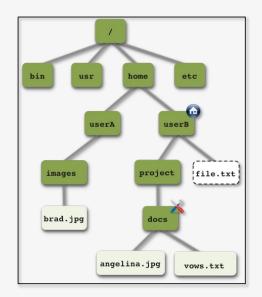
Copy brad.jpg to current directory

../../home/userA/images/brad.jpg

Navigation

cd

- for 'change directory'
- allows to navigate through the directories

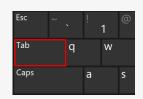


- o To go to the root: cd /
- To go to user home directory: cd ~ or just cd
- o To go up: cd ...
- o To go down: cd project/docs

Navigation – Auto-completion

Current working directory: home

$$[command] + 1x$$



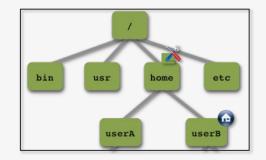


- Example: userA
 - userB





-> lists the content of the current directory



Navigation – Auto-completion

Fast navigation

Safe commands

Navigation – Content listing

Is

- for 'list'
- displays the directories and files of the current directory or of a specified directory

Options

- -I shows one item per line, with detailed information, such as dates and access rights
- -h prints file and directory sizes in human readable format (combined with -l)
- -a shows all files, including hidden files
- -t sorts by modification time (most recent first), default sorting being by name
- -r reverts sorting
- -R shows content recursively

Rules – case sensitivity

The command line differenciates upper from lower case letters:

brad.jpg

≠

BRAD.jpg

≠

brad.JPG

Rules – filename limitations

Nearly no limitation in length or characters. However...

- forbidden character: /
- not recommended characters:
 - characters with a particular meaning for the shell: space ,;: * ? & % \$ | ^ ~
 ' " () [] {}! \ #
 - international characters: é à æ ñ ç
- safe characters: _ . 0-9 a-z

Rules – filename extensions

File extensions are **arbitrary** and **do not have a particular meaning** for the operating system, but are useful for the users.

```
    .sh shell scripts
    .pl perl scripts
    .py python scripts
    .txt text files with no particular format
    .csv text files with Comma-Separated Values
    .fas files containing sequences in FASTA format*
```

*FASTA is a text-based format for representing either nucleotide or peptide sequences.

Rules – filename extensions

A file can have several extensions...

archive.tar.gz

archive.od.cw

...or no extension

tar = archive gz = compression



od = no meaning cw = no meaning

archive

Users and permissions

Every file / directory has access properties

who can access? 3 levels of classes:

user the file owner

group other users in the same group as the file owner

others all other users in the system

all users in the system

Users and permissions

Every file / directory has access properties

what kind of access? 3 access modes:

read permission to view the content of the file

write permission to edit the content of the file

execute permission to run a file (scripts, programs) or to

enter a directory

Users and permissions

Every file / directory has access properties

what restriction/permission?

- + adds the permission
- removes the permission
- applies the specified mode to the specified classes (faster if heterogeneous initial modes)

Root or system administrator has all rights!!!

chmod

```
chmod [u g o a] [+ - =] [r w x] file_name

____user
____group
____write
execute
```

Option:

-R recursive action

chmod can be run by root or by file owner only

```
-rwxrwxrwx file01.txt
-rwxrwxrwx file02.txt
```

How to allow everyone to read these files, but prevent 'group' + 'others' to 'write' and 'execute' them?

```
chmod go-wx file01.txt file02.txt
```

```
-rwxr--r-- file01.txt
-rwxr--r-- file02.txt
```

```
-rwxrwx--- file01.txt
-rwxr-xr-x file02.txt
```

How to allow everyone to read these files, but prevent 'group' + 'others' to 'write' and 'execute' them?

When several files with different permissions, it will be useful to set exact permissions using '='

```
chmod u=rwx,go=r-- file01.txt file02.txt
```

```
-rwxr--r-- file01.txt
-rwxr--r-- file02.txt
```

Each configuration of permission can be replaced by a code.

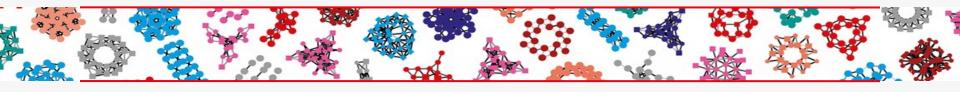
For example *chmod 700* = all permissions for owner, but none for all others ugo

Number	Octal Permission Representation	Ref
0	No permission	
1	Execute permission	X
2	Write permission	-W-
3	Execute and write permission: 1 (execute) + 2 (write) = 3	-wx
4	Read permission	r
5	Read and execute permission: 4 (read) + 1 (execute) = 5	r-x
6	Read and write permission: 4 (read) + 2 (write) = 6	rw-
7	All permissions: 4 (read) + 2 (write) + 1 (execute) = 7	rwx

In a nutshell

- Files and directories are organised as a tree
 - Navigate along its branches with cd
 - List folders content with Is
- Commands are executed at the current working directory if a path is not specified
- Rules
 - Case sensitivity
 - Filename extensions are arbitrary
 - Characters with a meaning for the shell are not recommended
- Access permissions for reading, writing and execution

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Exercises are integrated in chapters

Environment, processes & Jobs







User environment

man

Equivalent to help, often used to search commands' options

uname

Prints information about the system (several options)

whoami, id, groups, who

Prints information of the user

User environment

clear

This command allows to clean the screen

history

Allows to view the history of previous commands, which are listed with an increasing number

Call the last command with: !!

Search a string with ctrl + r

Browse history with up and down arrows

View page by page history with history | less

Browse through the last commands with the UP and DOWN keys

Alias

Regularly used complex commands can be renamed for simplification

Example:

alias la="ls -altr"

(list the content, including hidden files, ordered by reverse date)

- active only during the current session
- write it in a special file to make it permanent

Job status

- Run in the foreground
 - prompt not available until the job ends
 - the output is displayed on the terminal
- Run in the background
 - add & after the command
 - the prompt remains available
 - the output is not displayed on the terminal
- Done
- Stopped
- Terminated / killed -> (CTRL -c, kill)
 - when a process does not behave as expected frozen, gone into a loop...
 - Use CTRL -c when in foreground to kill the current process
 - Use kill %[jobID] to kill a job in background

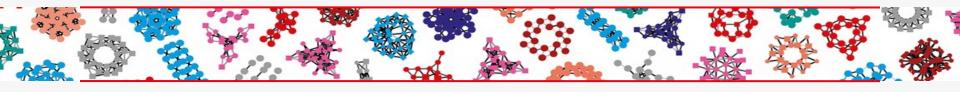




In a nutshell

- Commands to get information about you and your environment
- History of the last previous commands
- Simplfy commands with alias
- Jobs can be running in foreground or background
- Kill a process / job with CTRL -c when you get stuck

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Working with directories and files







Wildcard characters

are very useful for multiple files manipulation

```
*
     matches any number of characters in a file or directory name
     ls image*.jpeg ls *.jp*g
     matches exactly one character - use '??' to match any group of 2 characters
     1s *.???
     specify a range of characters allowed at that position – separated by an
     hyphen; use '!' to exclude a range of characters at that position
     ls [a-f]* ls [!a-f]*
     specify a list of terms - separated by commas
     ls *{.html,.txt}
```

mkdir

• "make directory": **creates** a new directory in the current directory mkdir new-directory(ies)

Option

-to create:

- several levels at a time: option –p
- several directories at a time with a path:
 mkdir level1/{level2a,level2b,level2c}
- several level with several directories
 mkdir -p 11/{L2a,L2b,L2c}

moves a file or a directory to a new location
 mv file-or-directory-name new-location/

renames a file or a directory
 mv file-or-directory-name new-name

Important: Moving files can overwrite existing files. -i option ask before overwritting



mv file1 file2

If no file2, file1 is renamed

If file2 exists, it's overwritten -> use option -i for confirm.



mv file1 directory2/ file1 is moved to directory2

mv file1 directory2 file1 is renamed directory2

Good Practice: autocompletion is useful to check if the new name or the new location exist

cp

- to make a <u>copy</u> of a file with another name cp file-name.txt file-name2.txt
- to make a copy of a file in another directory (same name is kept)
 cp file-name.txt Other_directory/
- to copy a directory and all its files
 cp -R directory/ new-directory/

Important: Copying files can overwrite existing files. Use option -i

rm

• to remove/delete a file rm file-name.txt

rmdir

• to remove/delete a directory rmdir empty-directory-name/

Important: by default a directory must be empty before it can be deleted.

rm options

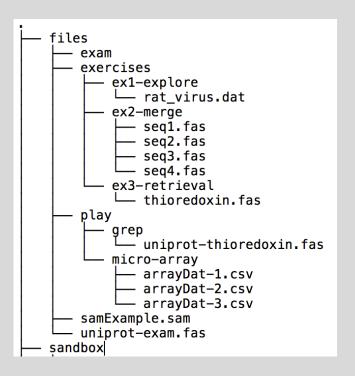
- -R or -r (for 'recursive')
 removes directories and their contents recursively
 rm -R non-empty-directory-name/
- -f (for '-force')
 never prompts for user confirmation, when files are writeprotected

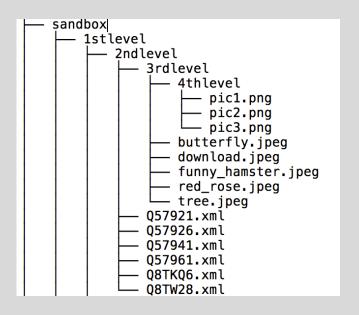
Use these options with care as there is no way back!

Hint: before executing a *rm* command with file names containing wildcard characters, simulate it first with the *ls* command as a control.

File organization

tree





Find files or directories

find

 Very effective in finding files & directories find [path] [query type] 'query term'

Path

- '.' to search in the current directory and its sub-directories
- '/' (root directory) to search in all directories
- Use single or multiple '.../' to search in parent directories
- '~' to search in your home directory

Find files or directories

Query types

- -name for a search based on the file name
 - **-iname** same but case insensitive

```
find . -name '*.java'
```

- -type f or -type d to limit the search to files only or directories only
- -size [+,-]n[scale], for a search based on the file size, where...
 + stands for 'larger than', for 'smaller than', nothing for 'exact size',
 n indicates the numeric value,
 scale indicates the size: c for bytes; k for kilobytes; M for megabytes and G for gigabytes

```
find \cdot -size +50M
```

• -perm [permission code]

```
find . -perm 644
```

Find files or directories

Tips

- Better to quote the query term with simple quotes
- Wildcards are possible
- ! placed after the path is the negative ("that do no match the criteria")
- Options can be combined
- Boolean operators (AND, OR) can be used in combination with find

```
find . -name '*.mpeg' -and -size +30M (default)
find . -name '*.png' -or -name '*.jpg'
find . \( -name '*.png' -or -name '*.jpg' \)
-and -size +30M
```

When multiple arguments, possible to use regular expressions (-regex option)

File type determination

Reminder: file extensions do not have a particular meaning for the OS, thus might not correspond to the real file format

file

To check the **format** and detailed information of a file: *file filename(s)*

- text the file contains only printing characters and a few common control characters
- executable the file contains the result of compiling a program
- data anything else (data is usually binary or non-printable)

New file

touch

 creates a **new** empty file touch filename(s)

If *filename* already exists, this command does not erase file content, but updates its latest modification time

Archiving and extracting data

tar

Creates, updates or expands archives

Options

- -z compresses using gzip program
- **-c** creates an archive
- -x extracts from an archive
- displays archive content (but does not extract it)
- -v displays information on the terminal window
- **-f** uses specified file
- set the current dates to extracted files

type of action

Archiving and extracting data

Highly recommended filename extensions:

- .tar for all archives
- .gz for gzip compressed archives

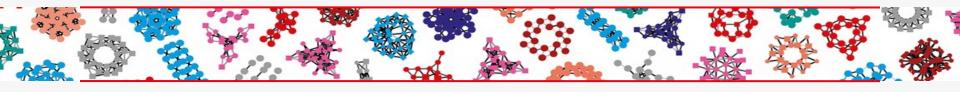
Tip: -f option must be placed at the last position because it requires argument (file name)

In a nutshell

- Directory and file manipulation
 - mkdir, mv, cp, rm, rmdir
- Finding files and directories (find)
 - Wildcards characters for file search and display
- File determination (file)

Archiving/extracting files (tar)

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Working with file content







Line by line

Rule:

Content search is performed line by line

File content statistics

WC

wc option filename(s)

Options

- -I prints the number of lines
- -w prints the number of words
- -c prints the number of bytes
- -m prints the number of characters

Without options, **wc** outputs the number of lines, words and bytes

File content display: head & tail

head

aims at quickly showing the beginning of a file

```
head myfile.txt -> displays the first 10 lines (default)
head -2 myfile.txt -> displays the first 2 lines
head -n-2 myfile.txt -> displays all the lines, except the last 2
```

tail

• is similar to **head**, but shows the **last lines** of a file

```
tail myfile.txt -> displays the last 10 lines

tail -2 myfile.txt -> displays the last 2 lines

tail -n+2 myfile.txt -> displays all lines except the first (useful e.g. to remove header line)
```

File content display: cat & less

cat displays the content of a text file

When several files are passed as arguments, cat concatenates and displays their content, thus can be used to merge the content of several files

File content display: cat & less

less

displays the content of a text file one screen at a time

Option

-N shows line numbers at the left of each line

Useful commands to be used inside the text file:

- [space-bar], shows the next page, one screen at a time
- up/down arrow keys, moves the content backward/forward one line at a time
- < and > to reach the beginning and the end of the document
- /mouse: search the string "mouse"
- **q** to quit

Text editors

Interactive use -> no need for text edition

Programmning -> need for text edition

Several programs available: Sublime Text, Visual Studio Code, etc

Vim is a text editor integrated into most terminals

Nano

UNIX has three standard streams

- Standard input stdin, where programs receive data from:
 - from the keyboard
 - from a file (using <)
- **Standard output stdout**, where programs write their output data to:
 - **printed** on the terminal window
 - written in a file (using > or >>)

- Standard error stderr, to output error messages
 - **printed** on the terminal window

Example of **standard input** from file

< not mandatory with most programs

Example of standard output to a file

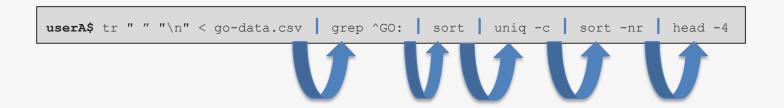
Command > filename

- if the file does not exist, it is created
- If it does, its content is overwritten

Command >> filename

- if the file does not exist, it is created (same function as >).
- If it does, the output is **added at the end** of the file content.

Output redirection: the | (pipe):



useful to pass directly the output from one program as the input of another without creating intermediate files

Delimiter-Separated Values (DSV)

Free-text (not DSV)

Hello, I will be very busy the next couple of months: I started a course in Bioinformatics!

Comma/Semicolon-separated values (CSV)

```
Entry, Entry_name, Protein_names
Q8QMT5, A18_CWPXB, Transcript termination protein A18
Q80DV6, A18_CWPXG, Transcript termination protein A18
```

Tab-separated values (TSV)

```
Entry Entry name Protein name

Q8QMT5 A18_CWPXB Transcript termination protein

A18 Q80DV6 A18_CWPXG Transcript termination

protein A18
```

text identification, retrieval and manipulation is more efficient when structured with delimiters

Delimiter-Separated Values (DSV)

Biological sequences are often represented in a so-called **FASTA** format:

- a first line starting with '>' and free text / comments (header line)
- main lines composed of one-letter code sequences

>sp|Q1PE49|40N1_ARATH Protein At-4/1 OS=Arabidopsis thaliana MAATSDEQMNLLLSSFDQIYEDFKIGLNEINVYRSKSNVESSRREVLEISNKNLKEENER LKKLYTESLNNFADQLEHRTKCHSLKEELKRVNDENKSKEHEHRNALESLRQKHVTKVEE

Newline character

structured formats → a 'newline' character* at the end of each line, which IS NOT the same for all OS

- \n -> Unix, Mac OS X
- \r -> Mac OS (before X)
- \r\n -> Windows OS

*use command *od -c* to view them

conversion is sometimes necessary

Converting file content

To convert newline characters...

tr (for 'translate') can do this in a single command line:

tr '\r' '\n' < myfile > mynewfile

tr is very convenient to change a delimiter, e.g. from TSV to CSV

If you want to replace words or phrases, the command **sed** is required (not discussed during this course)

Sorting file content

sort

- used to sort lines of text files
- default is alphabetical order

Options

- -n for a numeric sort
- **-r** for reverse sort
- -u for unique lines (keeps one instance when identical lines)
- -k sorts via a key (a column number for example)
- -t to define a key separator (e.g. a |). Default is space, but tab is recognized too

sort -k is useful if you want to sort according to only some parts of a line, typically columns

Searching / filtering file content

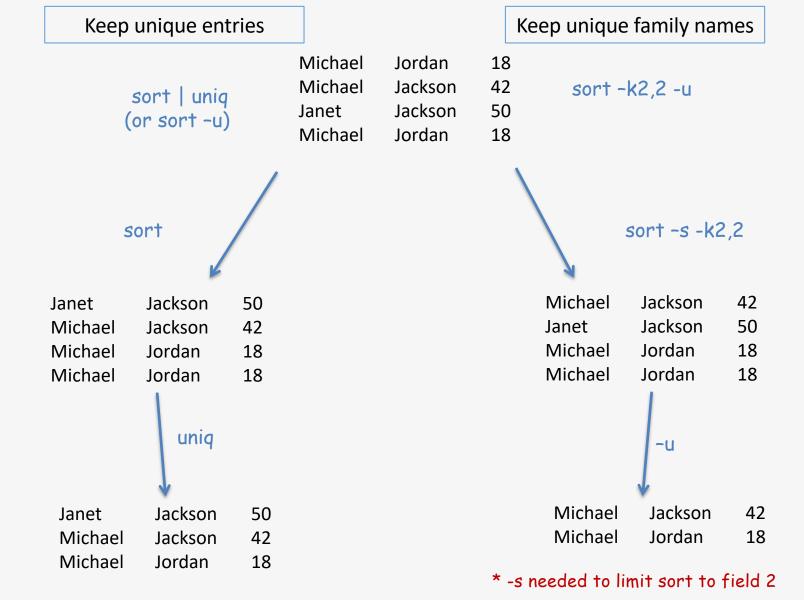
uniq

 reports unique lines by suppressing multiple occurrences of identical lines if sequential.
 Therefore, it is typically used after sort

Options

- -d, outputs only lines that are repeated (duplicated or more) in the input
- -c, precedes each reported line with the number of occurrences found
- -i, ignores the differences in case when comparing the lines
- -u, only prints unique lines

sort | uniq and sort -u have the same function: suppression of multiple occurrence of identical lines and ordering, but sort has an option (-k) to sort on specific key (e.g. a column) instead of the entire line.



Filtering / extracting file content

cut is used to extract selected parts of lines (like columns). Convenient to manipulate delimiter-separated value files

Options

- -c, selection based on characters positions. This is used when cut has to be performed at a fixed position (e.g. to remove a fixed header)
- -d, type of delimiter (default is 'tab'), e.g. ';' ',' ' or any character
- -f, selection based on fields in DSV files.
 single field number (e.g. -f 1), multiple field numbers (e.g. -f 1,4) or a range (e.g. -f 1-4) must be indicated. Fields are determined by delimiters if not TAB

NB: cut -f 1 | sort -u and sort -k1,1 -u are almost identical but the former will display only the extracted column

Comparing file content

diff compares 2 files and outputs the differences.

Useful to compare:

- 2 files with the same name in different directories
- different versions of the same file

Options

- -b, ignores differences in amount of white space
- -B, ignore differences of blank lines
- -s, reports when two files are identical (it does not by default)
- -q, reports only whether two files differ, no details of the differences

Merging file content

cat

- display function -> can be used to concatenate content from several files
- concatenation does not include any blank or newline

Options

- -s , squeezes multiple adjacent empty output lines
- -b, numbers nonempty output lines

paste

can merge columns from different files

Options

-d allows to introduce delimiters between columns (':' ',' '-')

Searching file content

grep

 for Global Regular Expression Print - searches file(s) for words or patterns and return matching lines grep [options] 'pattern' file(s)

Options

- -c, displays the number of resulting lines instead of the lines themselves
- -i, performs a case insensitive search
- -v, displays lines that DO NOT match the pattern
- -o, returns only the pattern, not the entire line
- -n, adds the line number in front of the result lines
- -r, search all files recursively inside each directory

Regular Expressions

Characters used to search a pattern, example:

^ a	'a' at the beginning of a line
a\$	'a' at the end of a line
^\$	to express a blank line
^.\$	any character on a line
[abc]	either character
[a-z]	a lowercase character
[0-9]	any figure
[0-59]	0, 1, 2, 3, 4, 5 or 9
[^0-9]	any character except a figure

In a nutshell

- UNIX allows to manipulate file content, such as order lines, cut fields, merge file content
- UNIX allows complex searches to retrieve filtered data
- Complex commands might be written into scripts
- Note that other languages are better suited to this sort of complex manipulations, like AWK, perl, python, or R

Next step

UNIX shell scripting in Life Sciences
By Thomas Junier & Robin Engler
13-15 June 2023
Lausanne

https://www.sib.swiss/training/course/20230606_ADVUN

Further resources

Our e-learning tutorial:

https://edu.sib.swiss/course/view.php?id=82

Resources that could be of interest:

http://en.wikipedia.org/wiki/List_of_Unix_commands

http://www.catonmat.net/projects/cheat-sheets/

https://ubuntudanmark.dk/filer/fwunixref.pdf

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